This article is showing a geometric and intuitive explanation of the covariance matrix and the way it describes the shape of a data set. We will describe the geometric relationship of the covariance matrix with the use of linear transformations and eigendecomposition.

Introduction

Before we get started, we shall take a quick look at the difference between covariance and variance. Variance measures the variation of a single random variable (like the height of a person in a population), whereas covariance is a measure of how much two random variables vary together (like the height of a person and the weight of a person in a population). The formula for variance is given by

$$\sigma_x^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

where n is the number of samples (e.g. the number of people) and $\bar{x}$ is the mean of the random variable x (represented as a vector). The covariance $\sigma(x, y)$ of two random variables x and y is given by

$$\sigma(x, y) = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

with n samples. The variance σ_x^2 of a random variable x can be also expressed as the covariance with itself by $\sigma(x, x)$.

Covariance Matrix

With the covariance we can calculate entries of the covariance matrix, which is a square matrix given by $C_{i,j} = \sigma(x_i, x_j)$ where $C \in \mathbb{R}^{d \times d}$ and d describes the dimension or number of random variables of the data (e.g. the number of features like height, width, weight, ...). Also the covariance matrix is symmetric since $\sigma(x_i, x_j) = \sigma(x_j, x_i)$. The diagonal entries of the covariance matrix are the variances and the other entries are the covariances. For this reason, the covariance matrix is sometimes called the _variance-covariance matrix_. The calculation for the covariance matrix can be also expressed as

$$C = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})(X_i - \bar{X})^T$$

$$\begin{array}{c|c|c|} & x & y \\ \hline x & \sigma_x^2 & \sigma(x,y) \\ \hline y & \sigma(y,x) & \sigma_y^2 \\ \hline \end{array}$$

where our data set is expressed by the matrix $X \in \mathbb{R}^{n \times d}$. Following from this equation, the covariance matrix can be computed for a data set with zero mean with $C = \frac{XX^T}{n-1}$ by using the semi-definite matrix XX^T .

In this article, we will focus on the two-dimensional case, but it can be easily generalized to more dimensional data. Following from the previous equations the covariance matrix for two dimensions is given by

$$C = \begin{pmatrix} \sigma(x, x) & \sigma(x, y) \\ \sigma(y, x) & \sigma(y, y) \end{pmatrix}$$

We want to show how linear transformations affect the data set and in result the covariance matrix. First we will generate random points with mean values $\bar{x}$, $\bar{y}$ at the origin and unit variance $\sigma_x^2 = \sigma_y^2 = 1$ which is also called [white noise](https://en.wikipedia.org/wiki/White_noise) and has the identity matrix as the covariance matrix.

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

plt.style.use('ggplot')
plt.rcParams['figure.figsize'] = (12, 8)

# Normal distributed x and y vector with mean 0 and standard deviation 1
x = np.random.normal(0, 1, 500)
y = np.random.normal(0, 1, 500)
X = np.vstack((x, y)).T

plt.scatter(X[:, 0], X[:, 1])
plt.title('Generated Data')
plt.axis('equal');
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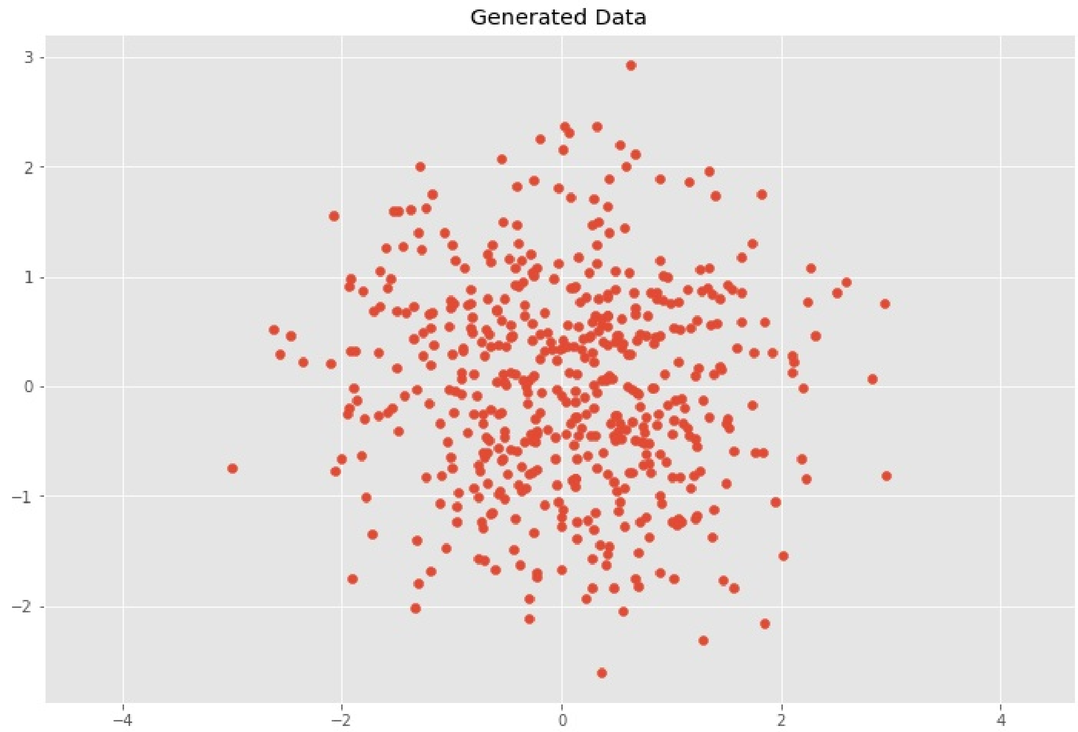
mean of X : $\frac{1}{n}\sum_{i=1}^{n} x_i$

standard deviation measures the amount of variation or dispersion of a set of values
low standard deviation $\longrightarrow$ values are closer to the mean



This case would mean that x and y are independent (or uncorrelated) and the covariance matrix C is

$$C = \begin{pmatrix} \sigma_x^2 & 0 \\ 0 & \sigma_y^2 \end{pmatrix}$$

We can check this by calculating the covariance matrix

```
# Covariance
def cov(x, y):
    xbar, ybar = x.mean(), y.mean()
    return np.sum((x - xbar)*(y - ybar))/(len(x) - 1)

# Covariance matrix
def cov_mat(X):
    return np.array([[cov(X[0], X[0]), cov(X[0], X[1])], \
                     [cov(X[1], X[0]), cov(X[1], X[1])]])

# Calculate covariance matrix
cov_mat(X.T) # (or with np.cov(X.T))
array([[ 1.008072  , -0.01495206],
       [-0.01495206,  0.92558318]])
```

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Which approximatelly gives us our expected covariance matrix with variances $\sigma_x^2 = \sigma_y^2 = 1$.

Linear Transformations of the Data Set

Next, we will look at how transformations affect our data and the covariance matrix C . We will transform our data with the following scaling matrix.

$$S = \begin{pmatrix} s_x & 0 \\ 0 & s_y \end{pmatrix}$$

where the transformation simply scales the x and y components by multiplying them by s_x and s_y respectively. What we expect is that the covariance matrix C of our transformed data set will simply be

$$C = \begin{pmatrix} (s_x\sigma_x)^2 & 0 \\ 0 & (s_y\sigma_y)^2 \end{pmatrix}$$

which means that we can extract the scaling matrix from our covariance matrix by calculating $S = \sqrt{C}$ and the data is transformed by $Y = SX$.

```
# Center the matrix at the origin
X = X - np.mean(X, 0)

# Scaling matrix
sx, sy = 0.7, 3.4
```

```
Scale = np.array([[sx, 0], [0, sy]])

# Apply scaling matrix to X
Y = X.dot(Scale)

plt.scatter(Y[:, 0], Y[:, 1])
plt.title('Transformed Data')
plt.axis('equal')

# Calculate covariance matrix
cov_mat(Y.T)
array([[ 0.50558298, -0.09532611],
       [-0.09532611, 10.43067155]])
```

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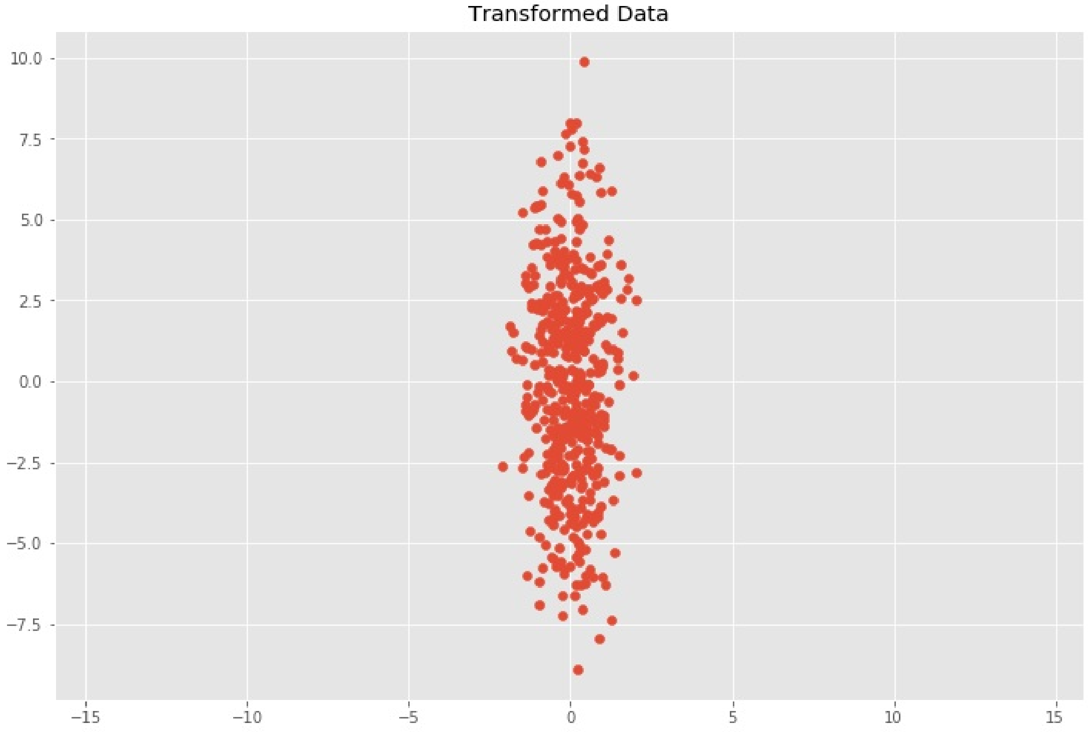

We can see that this does in fact approximately match our expectation with $0.7^2 = 0.49$ and $3.4^2 = 11.56$ for $(s_x\sigma_x)^2$ and $(s_y\sigma_y)^2$. This relation holds when the data is scaled in x and y direction, but it gets more involved for other linear transformations.

Now we will apply a linear transformation in the form of a transformation matrix T to the data set which will be composed of a two dimensional [rotation matrix](https://en.wikipedia.org/wiki/Rotation_matrix) R and the previous scaling matrix S as follows

$$T = RS$$

where the rotation matrix R is given by

$$R = \begin{pmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{pmatrix}$$

where θ is the rotation angle. The transformed data is then calculated by $Y = TX$ or $Y = RSX$.

```
# Scaling matrix
sx, sy = 0.7, 3.4
Scale = np.array([[sx, 0], [0, sy]])

# Rotation matrix
theta = 0.77*np.pi
c, s = np.cos(theta), np.sin(theta)
Rot = np.array([[c, -s], [s, c]])

# Transformation matrix
T = Scale.dot(Rot)

# Apply transformation matrix to X
Y = X.dot(T)

plt.scatter(Y[:, 0], Y[:, 1])
plt.title('Transformed Data')
plt.axis('equal');

# Calculate covariance matrix
```

```
cov_mat(Y.T)
array([[ 4.94072998, -4.93536067],
       [-4.93536067,  5.99552455]])
```

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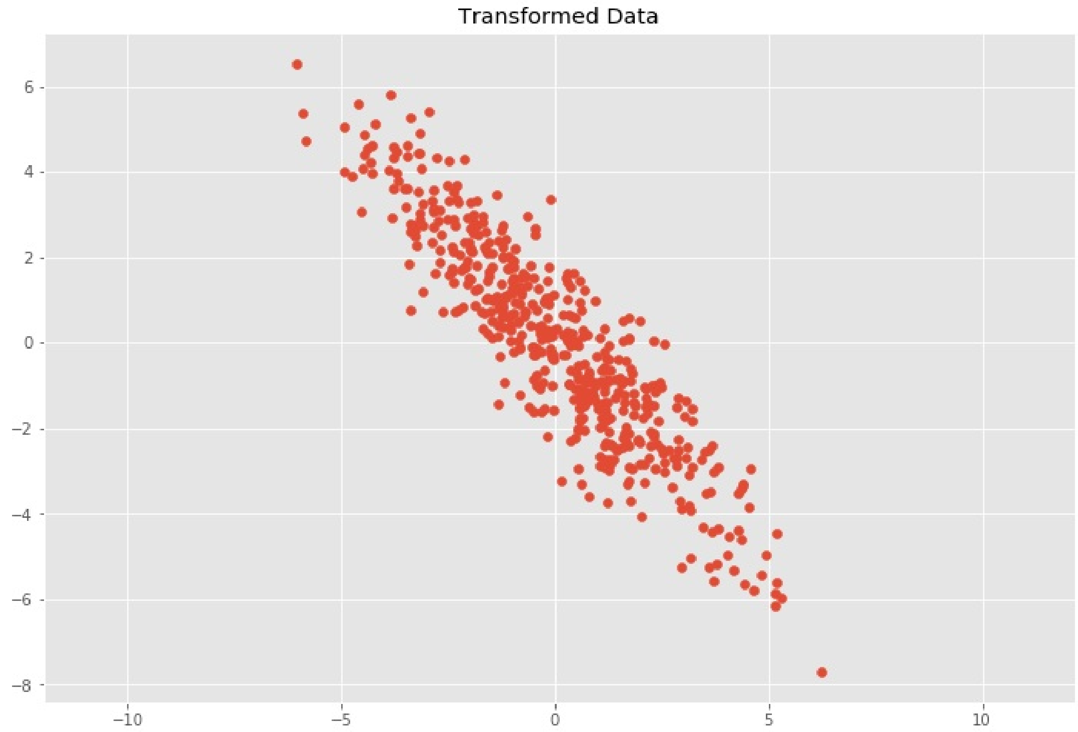

This leads to the question of how to decompose the covariance matrix C into a rotation matrix R and a scaling matrix S .

Eigen Decomposition of the Covariance Matrix

Eigen Decomposition is one connection between a linear transformation and the covariance matrix. An eigenvector is a vector whose direction remains unchanged when a linear transformation is applied to it. It can be expressed as

$$Av = \lambda v$$

where v is an eigenvector of A and λ is the corresponding eigenvalue. If we put all eigenvectors into the columns of a Matrix V and all eigenvalues as the entries of a diagonal matrix L we can write for our covariance matrix C the following equation

$$CV = VL$$

where the covariance matrix can be represented as

$$C = VLV^{-1}$$

which can be also obtained by [Singular Value Decomposition](). The eigenvectors are unit vectors representing the direction of the largest variance of the data, while the eigenvalues represent the magnitude of this variance in the corresponding directions. This means V represents a rotation matrix and $\sqrt{L}$ represents a scaling matrix. From this equation, we can represent the covariance matrix C as

$$C = RSSR^{-1}$$

where the rotation matrix $R = V$ and the scaling matrix $S = \sqrt{L}$. From the previous linear transformation $T = RS$ we can derive

$$C = RSSR^{-1} = TT^T$$

because $T^T = (RS)^T = S^T R^T = SR^{-1}$ due to the properties $R^{-1} = R^T$ since R is orthogonal and $S = S^T$ since S is a diagonal matrix. This enables us to calculate the covariance matrix from a linear transformation. In order to calculate the linear transformation of the covariance matrix, one must calculate the eigenvectors and eigenvectors from the covariance matrix C . This can be done by calculating

$$T = V\sqrt{L}$$

where V is the previous matrix where the columns are the eigenvectors of C and L is the previous diagonal matrix consisting of the corresponding eigenvalues. The transformation matrix can be also computed by the [Cholesky decomposition]() with $Z = L^{-1}(X - \bar{X})$ where L is the Cholesky factor of $C = LL^T$.

We can see the basis vectors of the transformation matrix by showing each eigenvector v multiplied by $\sigma = \sqrt{\lambda}$. By multiplying σ with 3 we cover approximately 99.7% of the points according to the three sigma rule if we would draw an ellipse with the two basis vectors and count the points inside the ellipse.

```
C = cov_mat(Y.T)
eVe, eVa = np.linalg.eig(C)

plt.scatter(Y[:, 0], Y[:, 1])
for e, v in zip(eVe, eVa.T):
    plt.plot([0, 3*np.sqrt(e)*v[0]], [0, 3*np.sqrt(e)*v[1]], 'k-', lw=2)
plt.title('Transformed Data')
plt.axis('equal');
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```

We can now get from the covariance the transformation matrix T and we can use the inverse of T to remove correlation (whiten) the data.

```
C = cov_mat(Y.T)

# Calculate eigenvalues
eVa, eVe = np.linalg.eig(C)

# Calculate transformation matrix from eigen decomposition
R, S = eVe, np.diag(np.sqrt(eVa))
T = R.dot(S).T

# Transform data with inverse transformation matrix T^-1
Z = Y.dot(np.linalg.inv(T))

plt.scatter(Z[:, 0], Z[:, 1])
plt.title('Uncorrelated Data')
plt.axis('equal');

# Covariance matrix of the uncorrelated data
cov_mat(Z.T)
array([[ 1.00000000e+00, -1.24594167e-16],
       [-1.24594167e-16,  1.00000000e+00]])

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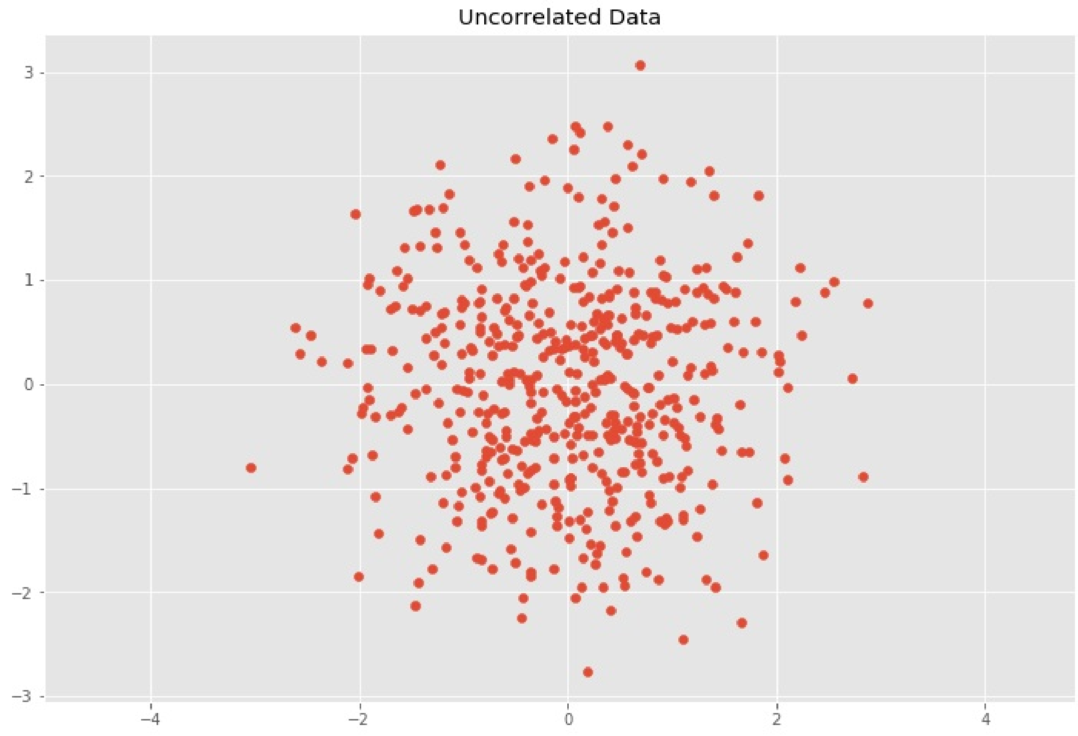

An interesting use of the covariance matrix is in the Mahalanobis distance, which is used when measuring multivariate distances with covariance. It does that by calculating the uncorrelated distance between a point x to a multivariate normal distribution with the following formula

$$D_M(x) = \sqrt{(x-\mu)^T C^{-1}(x-\mu))}$$

where μ is the mean and C is the covariance of the multivariate normal distribution (the set of points assumed to be normal distributed). A derivation of the Mahalanobis distance with the use of the Cholesky decomposition can be found in this article.